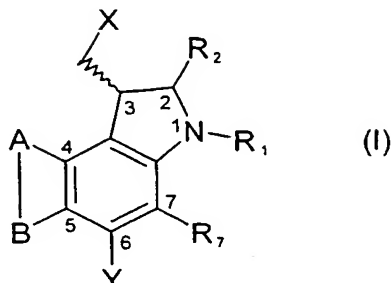


CLAIMS

1. A compound of formula I:



wherein:

X is an electrophilic leaving group;

Y is selected from NH-Prot, O-Prot, S-Prot, NO₂, NHOH, N₃, NHR, NRR, N=NR, N(O)RR, NHSO₂R, N=NPhR, SR or SSR, where Prot represents a protecting group;

A and B collectively represent a fused benzene or pyrrole ring (in either orientation), which is optionally substituted by up to respectively 4 or 2 groups independently selected from R, OH, OR, halo, nitro, amino, Me₃Sn, CO₂H, CO₂R;

R₁ is a nitrogen protecting group, where if Y includes a protecting group, these protecting groups are orthogonal;

R₂ and R₇ are independently selected from H, R, OH, OR, halo, nitro, amino, Me₃Sn;

wherein R is selected from:

(a) a lower alkyl group having 1 to 10 carbon atoms,

(b) an aralkyl group (i.e. an alkyl group with one or more aryl substituents), preferably of up to 12 carbon atoms;

the alkyl group of (a) or (b) optionally containing one or more carbon-carbon double or triple bonds, which may form part of a conjugated system; and

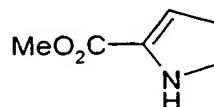
(c) an aryl group, preferably of up to 12 carbon atoms;

and wherein:

R is optionally substituted by one or more halo, hydroxy, amino, or nitro groups, and optionally

contains one or more hetero atoms, which may form part of, or be, a functional group;

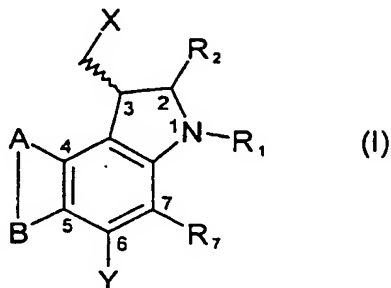
except that when R_1 is Boc, Y is NO_2 , X is Cl, and R_2 and R_7 are H, then A and B do not collectively represent either an unsubstituted benzene ring or:



2. A compound according to claim 1, wherein R is independently selected from a lower alkyl group having 1 to 10 carbon atoms, or an aralkyl group, preferably of up to 12 carbon atoms, or an aryl group, preferably of up to 12 carbon atoms, optionally substituted by one or more halo, hydroxy, amino, or nitro groups.
3. A compound according to claim 2, wherein R is independently selected from lower alkyl groups having 1 to 10 carbon atoms optionally substituted by one or more halo, hydroxy, amino, or nitro groups.
4. A compound according to claim 3, wherein R is an unsubstituted straight or branched chain alkyl group, having 1 to 10 carbon atoms.
5. A compound according to any one of the preceding claims, wherein R_1 has a carbamate functionality where it binds to the nitrogen atom of the CPI.
6. A compound according to any one of the preceding claims, wherein Y is NH-Prot, O-Prot or S-Prot.
7. A compound according to claim 6, wherein Y is NH-Prot.
8. A compound according to any one of the preceding claims, wherein X is either halogen or OSO_2R .

CLAIMS

1. A ~~Combination unit~~ ~~[Compound]~~ of formula I:



(substituted by a CO_2R or CO_2H group and is further).

wherein:

X is an electrophilic leaving group;

Y is selected from NH-Prot, O-Prot, S-Prot, NO_2 , NHOH, N_3 , NHR, NRR, $\text{N}=\text{NR}$, $\text{N}(\text{O})\text{RR}$, NHSO_2R , $\text{N}=\text{NPhR}$, SR or SSR, where Prot represents a protecting group;

A and B collectively represent a fused benzene or pyrrole ring (in either orientation), which is optionally substituted by up to respectively ³ or ² group(s) independently selected from R, OH, OR, halo, nitro, amino, Me_3Sn , CO_2H , CO_2R ;

R_1 is a nitrogen protecting group, where if Y includes a protecting group, these protecting groups are orthogonal;

R_2 and R_7 are independently selected from H, R, OH, OR, halo, nitro, amino, Me_3Sn ;

wherein R is selected from:

(a) a lower alkyl group having 1 to 10 carbon atoms,

(b) an aralkyl group (i.e. an alkyl group with one or more aryl substituents), preferably of up to 12 carbon atoms;

the alkyl group of (a) or (b) optionally containing one or more carbon-carbon double or triple bonds, which may form part of a conjugated system; and

(c) an aryl group, preferably of up to 12 carbon atoms;

and wherein:

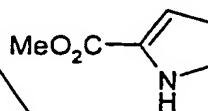
R is optionally substituted by one or more halo, hydroxy, amino, or nitro groups, and optionally

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55

contains one or more hetero atoms, which may form part of, or be, a functional group;

except that when R_1 is Boc, Y is NO_2 , X is Cl, and R_2 and R_7 are H, then A and B do not collectively represent either an unsubstituted benzene ring or:



10

combinatorial unit

2. A ~~compound~~ according to claim 1, wherein R is independently selected from a lower alkyl group having 1 to 10 carbon atoms, or an aralkyl group, preferably of up to 12 carbon atoms, or an aryl group, preferably of up to 12 carbon atoms, optionally substituted by one or more halo, hydroxy, amino, or nitro groups.

15

3. A compound according to claim 2, wherein R is independently selected from lower alkyl groups having 1 to 10 carbon atoms optionally substituted by one or more halo, hydroxy, amino, or nitro groups.

20

Sub
B1

combinatorial unit

4. A ~~compound~~ according to claim 3, wherein R is an unsubstituted straight or branched chain alkyl group, having 1 to 10 carbon atoms.

25

combinatorial unit

5. A ~~compound~~ according to any one of the preceding claims, wherein R_1 has a carbamate functionality where it binds to the nitrogen atom of the CPI.

30

combinatorial unit

6. A ~~compound~~ according to any one of the preceding claims, wherein Y is NH-Prot, O-Prot or S-Prot.

combinatorial unit

7. A ~~compound~~ according to claim 6, wherein Y is NH-Prot.

35

combinatorial unit

8. A ~~compound~~ according to any one of the preceding claims, wherein X is either halogen or OSO_2R .

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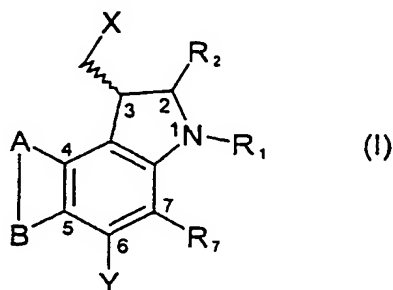
Sub
A3

combinatorial unit

56

9. A ~~compound~~ according to any one of the preceding claims, wherein the 4,5 fused ring is substituted by $-CO_2R$ in the 2 or 3 position if it is a benzene ring, or in the 2 position if it is a pyrrole ring.

10. The use of compounds of formula I:



wherein:

X is an electrophilic leaving group;

Y is selected from NH_2 , NH-Prot, OH, O-Prot, SH, S-Prot, NO_2 , NHOH, N_3 , NHR, NRR, $N=NR$, $N(O)RR$, $NHSO_2R$, $N=NPhR$, SR or SSR, where Prot represents a protecting group;

A and B collectively represent a fused benzene or pyrrole ring (in either orientation), which is optionally substituted by up to respectively 4 or 2 groups independently selected from R, OH, OR, halo, nitro, amino, Me_3Sn , CO_2H , CO_2R ;

R_1 is a nitrogen protecting group, where if Y includes a protecting group, these protecting groups are orthogonal;

R_2 and R_7 are independently selected from H, R, OH, OR, halo, nitro, amino, Me_3Sn ;

wherein R is selected from:

(a) a lower alkyl group having 1 to 10 carbon atoms,

(b) an aralkyl group (i.e. an alkyl group with one or more aryl substituents), preferably of up to 12 carbon atoms;

the alkyl group of (a) or (b) optionally containing one or more carbon-carbon double or triple bonds, which may form part of a conjugated system; and

(c) an aryl group, preferably of up to 12 carbon atoms;

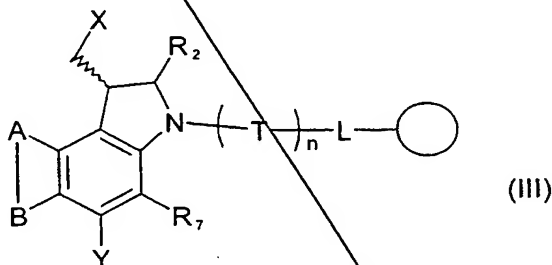
and wherein:

R is optionally substituted by one or more halo, hydroxy, amino, or nitro groups, and optionally contains one or more hetero atoms, which may form part of, or be, a functional group;

in methods of combinatorial chemistry synthesis, wherein the compound of formula I is joined to a solid support by a chain comprising at least one combinatorial unit.

11. The use according to claim 10, wherein Y is NH₂, NH-Prot, OH, O-Prot, SH, or S-Prot.

12. A compound of formula III:



wherein:

X, Y, A, B, R₂ and R₇ are as defined in claim 10;

T is a combinatorial unit;

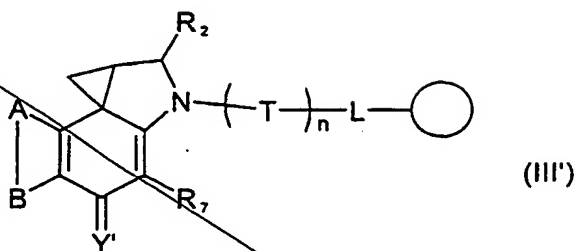
n is a positive integer, where if n is greater than 1, each T may be different;

L is a linking group, or less preferably a single bond; and,

O is a solid support.

58

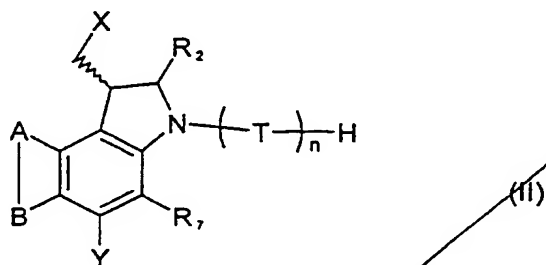
13. A compound of formula III':



wherein:

A, B, R₂, R₇, T, n, L and O are as defined in claim 12; and, Y' is NH, O or S.

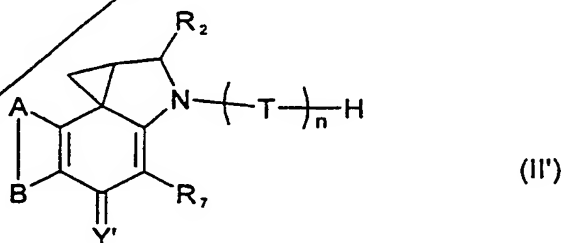
~~14. A compound of formula II:~~



wherein:

X, Y, A, B, R₂, R₇, T and n are as defined in claim 12.

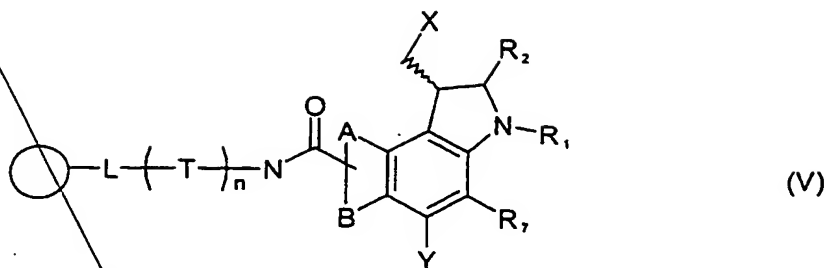
15. A compound of formula II':



wherein:

~~A, B, T, n, R₂, R₇ and Y' are as defined in claim 13.~~

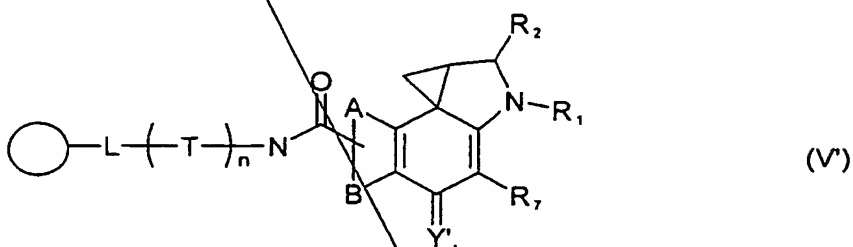
14 16. A compound of formula V:



wherein:

5 A, B, Y, R₁, R₂, and R₇, are as defined in claim 10; and, T, n, L and O are as defined claim 12.

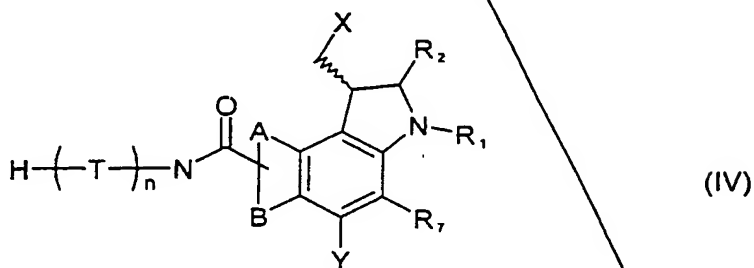
15 17. A compound of formula V':



wherein:

A, B, R₁, R₂, and R₇ are as defined in claim 10; and, T, n, L, Y' and O are as defined in claim 13.

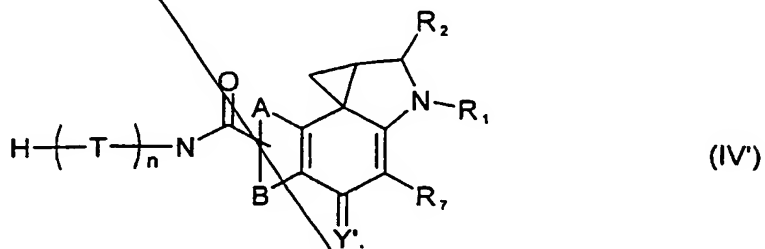
15 18. A compound of formula IV:



wherein:

20 A, B, X, Y, R₁, R₂ and R₇ are as defined in claim 10; and, T and n are as defined in claim 12.

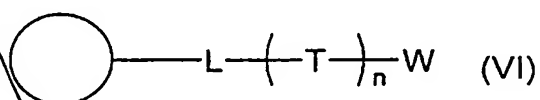
1719. A compound of formula IV':



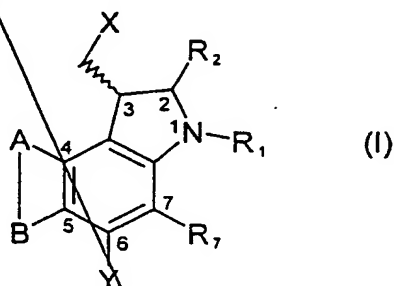
wherein:

A, B, T, n, R₁, R₂ and R₇ are as defined in claim 16; and, Y' is NH, O or S.

1820. A method of preparing a compound according to claim 12 by reaction of a compound of formula VI:



with a compound of formula I:

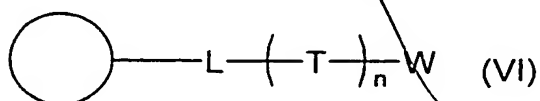


wherein:

A, B, R_2 , R_7 , T, n, ~~L~~ and O are as defined in claim 12;
and,

W is H or an atom or group for providing a functional group capable of reaction with $-NH_2$.

1921. A method of preparing a compound according to claim 16, by reaction of a compound of formula VI:



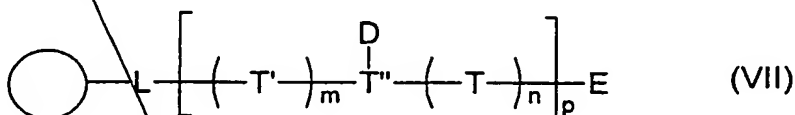
61

with a compound of formula I according to claim 10, where the 4,5 fused ring is substituted by $-CO_2R$ in the 2 or 3 position if it is a benzene ring, or in the 2 position if it is a pyrrole ring, and wherein:

T, n, L and O are as defined in claim 16; and,

W is H or an atom or group for providing a functional group capable of reaction with $-COOH$.

10 2022. A compound of formula VII:



wherein:

O, T, and L are as defined in ~~the~~ claim 12;

n and m are positive integers, or one of them may be zero;

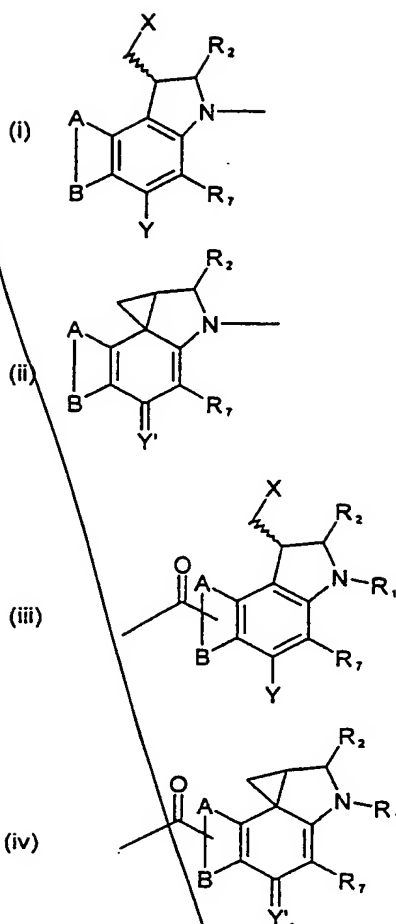
T' is a combinatorial unit, where each T' may be different if m is greater than 1;

T'' is a combinatorial unit which provides a site for the attachment of D;

D is selected from:

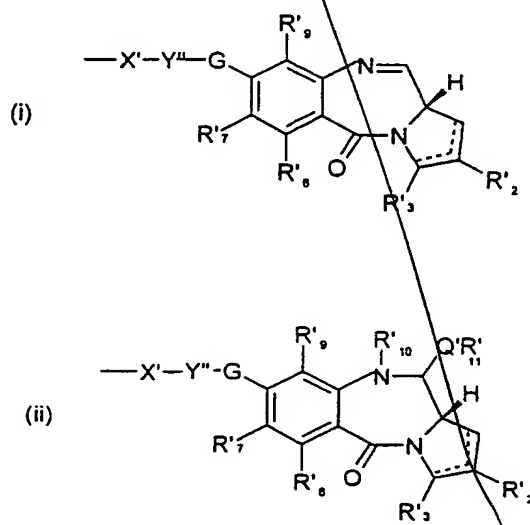
62

(a)



wherein A, B, Y, R₁, R₂ and R₇ are as defined in claim 11 and Y' is NH, NR, O or S;

(b)



wherein:

X' is selected from CO, NH, S, or O;

G is O, S, NH, or a single bond;

R'₂ and R'₃ are independently selected from: H, R, OH, OR, =O, =CH-R, =CH₂, CH₂-CO₂R, CH₂-CO₂H, CH₂-SO₂R, O-SO₂R, CO₂R, COR and CN, and there is optionally a double bond between C₂ and C₃;

R'₆, R'₇, and R'₉ are independently selected from H, R, OH, OR, halo, nitro, amino, Me₃Sn;

R'₁₁ is either H or R;

Q' is S, O or NH;

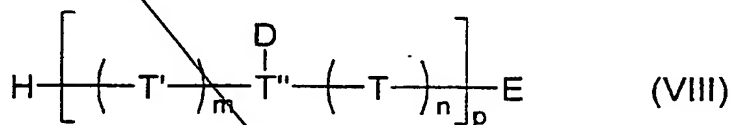
R'₁₀ is a nitrogen protecting group;

Y'' is a divalent group such that HY = R;

p is a positive integer, where if p is greater than 1, for each repeating unit, the meaning of T, T', T'' and D and the values of n and m are independently selected; and,

E is selected from the same possibilities as D; provided that at least one group D or E is selected from (a).

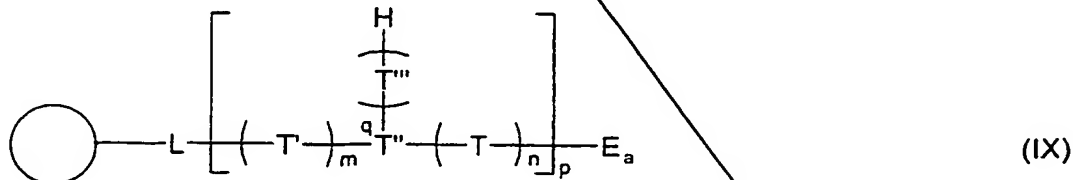
2123. A compound of formula (VIII):



wherein:

L, T, T', T'', D, E, n, m and p are as defined in claim 22.

2224. A compound of formula (IX):



wherein:

O, L, T, T', T'', n, m and p are as defined in claim 22;

T'' is a combinatorial unit;

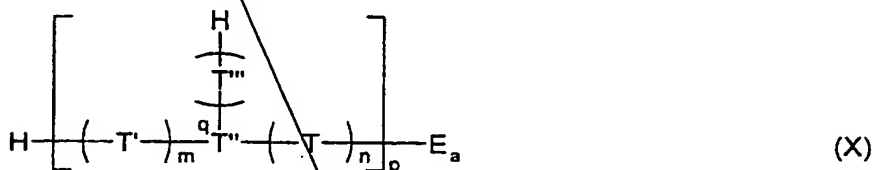
q is a positive integer, where if q is greater than 1, each T'' may be different; and,

E_a is selected from the group (a) of E as defined in claim 22;

wherein:

if p is greater than 1, for each repeating unit the meaning of T, T', T'', T''' and the values of n, m and q are independently selected.

23 25. A compound of formula (X):



wherein:

L, T, T', T'', T''', E_a, n, m, p and q are as defined in claim 22.

20 24 26. A collection of compounds all of which are represented by either:

(i) formula III as defined in claim 12;

(ii) formula III' as defined in claim 13;

~~(iii) formula II as defined in claim 14;~~

~~(iv) formula II' as defined in claim 15;~~

ⁱⁱⁱ
(v) formula V as defined in claim 18;

^{iv}
(vi) formula V' as defined in claim 17;

~~(vii)~~ formula IV as defined in claim 18;

~~(viii)~~ formula IV' as defined in claim 17;

^{vii}
(ix) formula VII as defined in claim 22;

^{viii}
(x) formula VIII as defined in claim 21;

^{ix}
(xi) formula IX as defined in claim 22; or,

~~(xii)~~ formula X as defined in claim 23.

²⁵
27. A method of preparing a collection of compounds as defined in claim ²⁴26.

²⁶
28. A method of screening compounds of:

- 5 ~~(i) formula II as defined in claim 14,~~
~~(ii) formula II' as defined in claim 15;~~
 (iii) formula IV as defined in claim ¹⁶18;
 (iv) formula IV' as defined in claim ¹⁷19;
 (v) formula VIII as defined in claim ²¹23; or,
 (vi) formula X as defined in claim ²³25;

to discover biologically active compounds.

²⁷
29. The use of a compound of:

- 15 ~~(i) formula II as defined in claim 14,~~
~~(ii) formula II' as defined in claim 15;~~
 (iii) formula IV as defined in claim ¹⁶18;
 (iv) formula IV' as defined in claim ¹⁷19;
 (v) formula VIII as defined in claim ²¹23; or
 (vi) formula X as defined in claim ²³25;

20 in the manufacture of a cytotoxic, antibiotic, antiparasitic or antiviral therapeutic composition.

²⁸
30. The use of a compound of:

- 25 (i) formula III as defined in claim 12;
 (ii) formula III' as defined in claim 13;
 (iii) formula V as defined in claim ¹⁴16;
 (iv) formula V' as defined in claim ¹⁵17;
 (v) formula VII as defined in claim ²⁰22; or,
 (vi) formula IX as defined in claim ²²24;

30 in a method of diagnosis.

²⁹
31. The use of a compound of:

- 35 ~~(i) formula II as defined in claim 14;~~
~~(ii) formula II' as defined in claim 15;~~
 (iii) formula IV as defined in claim ¹⁶18;
 (iv) formula IV' as defined in claim ¹⁷19;
 (v) formula VIII as defined in claim ²¹23; or,

66

23

^{iv}
~~(vi)~~ formula X as defined in claim ²³23;
 in a method of target validation.

30

³⁰
~~22.~~ The use of a compound of:

5

~~(i) formula II as defined in claim 14;~~

~~(ii) formula II' as defined in claim 15;~~

~~(iii) formula IV as defined in claim ¹⁶18;~~

~~(iv) formula IV' as defined in claim ¹⁷19;~~

~~(v) formula VIII as defined in claim ²¹23; or,~~

10

~~(vi) formula X as defined in claim ²³25;~~

in a method of functional genomics.

add
 B1